

Diluted Antiferromagnetic 3D Ising model in a field

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We present numerical simulations for the diluted antiferromagnetic 3D Ising model (DAFF) in an external magnetic field at zero temperature. Our results are compatible with the DAFF being in the same universality class as the Random Field Ising model, in agreement with the renormalization group prediction.

Despite numerous efforts phase transitions in disordered systems are not yet fully understood. In experiments it is difficult to reach thermal equilibrium. The same is true in many numerical simulations which face the additional difficulty of very large sample to sample fluctuations. It turns out that the random field Ising model (RFIM) is the only case where this difficulty can be overcome due to the possibility of finding exact ground states (no thermalisation problem), using a very fast algorithm [1, 2]. This allowed the simulation of very large systems with high statistics [1, 3–5]. On the theoretical side, the RFIM and the diluted branched polymers are the only models where renormalization group can be carried out to all orders of perturbation theory [6–8]. It predicts dimensional reduction in both cases. Here dimensional reduction means that the critical exponents of the RFIM in D dimensions are the same with the exponents of the ferromagnetic Ising model in $D - 2$ dimensions. Dimensional reduction has been proven true for the diluted branched polymers [9], while it is not true for the RFIM [10].

One of the most striking predictions of perturbative renormalization group (PRG) is that the RFIM and the diluted antiferromagnets in an external magnetic field (DAFF) are in the same universality class [11, 12]. This is very important because it allows the connection with experiments: there are no experimental realizations of the RFIM, while the DAFF has been studied experimentally extensively [16–18]. PRG universality predicts that critical exponents and other universal quantities (see later) take the same values for the RFIM and the DAFF and that they do not depend on the random field probability distribution for the RFIM or the dilution for the DAFF. The validity of this prediction is not guaranteed because other predictions of the PRG (dimensional reduction) are false. Indeed it has been speculated that the RFIM and the DAFF are not in the same universality class [13, 15].

In the present paper we establish numerically for the first time that the RFIM and the DAFF are in the same universality class and that universal quantities do not depend on the dilution probability in the DAFF as predicted by the PRG. It has been shown recently that in the case of the RFIM, different random field probability dis-

tributions of the random field belong to the same universality class [5]. No clear picture has yet emerged from the experimental studies. These results raise two questions: why some predictions of PRG are verified, while others are not, and why the critical exponents measured experimentally [16–18] are different for different experiments and from the values obtained by numerical simulations.

A very large number of numerical simulations have been devoted to the study of the RFIM. Much less effort has been devoted to the numerical study of the DAFF [13–15].

We start from the Ising antiferromagnet in a field :

$$\mathcal{H}_{AF} = J \sum_{\langle ij \rangle} \sigma_i \sigma_j - H_0 \sum_i \sigma_i ,$$

with the spins $\sigma_i = \pm 1$ on a cubic lattice of linear size L . We considered nearest neighbour interactions and periodic boundary conditions. H_0 is an external constant magnetic field. The coupling between spins is antiferromagnetic, *i.e.* $J > 0$. It is convenient to perform a gauge transformation $\sigma(x, y, z) \rightarrow (-1)^{x+y+z} \sigma(x, y, z)$. For a cubic lattice, periodic boundary conditions and even L we obtain, because of the absence of frustration, a ferromagnet in an alternating magnetic field

$$\mathcal{H}_{AF} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - H_0 \sum_i (-1)^{i_x+i_y+i_z} \sigma_i .$$

We will consider this model in the presence of random site dilution. For this we replace the spin variables σ_i with $\epsilon_i \sigma_i$ where ϵ_i are independent quenched random variables which take the value 0 with a probability d (dilution) or 1 with a probability $1 - d$. Then the Hamiltonian for a given configuration of dilution ϵ_i (instance) is

$$\mathcal{H}_{DAFF} = -J \sum_{\langle ij \rangle} \epsilon_i \epsilon_j \sigma_i \sigma_j - H_0 \sum_i (-1)^{i_x+i_y+i_z} \epsilon_i \sigma_i . \quad (1)$$

The relevant parameters of the DAFF are the temperature T and the ratio $R = H_0/J$. The phase diagram of the DAFF is a line in the $T - R$ plane. It is believed that all points on this line belong to the same universality class. This line crosses the $T = 0$ axis, *i.e.* there is

a phase transition at $T = 0$. It is well known that it is possible to find exact ground states of the ferromagnetic RFIM using a very fast optimisation algorithm [1, 2]. The properties of the phase transition of the RFIM have been studied by the extensive use of this algorithm [1–4, 13].

The goal of transforming the original Hamiltonian to the one of eq. (1) is to allow the use of this algorithm [13]. In this paper we present the results of extensive numerical simulations of the DAFF on a cubic lattice in three dimensions with periodic boundary conditions. We have studied the case of dilution probabilities, $d = 0, 05$, $d = 0.07$ and $d = 0.37$. Our results are compatible with universality for all three values of d . The renormalization group argument for universality is valid for small d , $d < d_c$, but there is no estimation of d_c . It has been speculated that d_c may be the percolation threshold $d_p = 0.3116077(4)$ [19]. We find universality even for $d = 0.37 > d_p$.

In order to locate the phase transition and extract the critical properties, we compute the ground state magnetization for different values of R and sizes L for a large number of samples, typically 10^6 . From the magnetization we compute the dimensionless Binder like magnetic cumulant U_4

$$U_4(R, L) = \frac{[m(R, L)^4]}{[m(R, L)^2]^2}, \quad (2)$$

where $[A]$ is the average of A over the samples. We also compute the dimensionless ratio $\xi(R, L)/L$, where ξ is the correlation length and L the system linear size. The correlation length is defined from the wave-vector susceptibility $\chi(\vec{k}) = \left[\langle (\sum_j \sigma_j e^{i\vec{k} \cdot \vec{r}_j})^2 \rangle \right] / N^2$ as [20] :

$$\xi = \frac{1}{2 \sin(\pi/L)} \sqrt{\frac{\chi(0)}{\chi(\vec{k}_{min})}} - 1, \quad (3)$$

with N the number of spins and $\vec{k}_{min} = (\frac{2\pi}{L}, 0, 0)$.

We compute the L dependant effective critical values of R , $R_{c,U}(L)$ and $R_{c,\xi}(L)$. $R_{c,U}(L)$ is the value of R for which $U_4(R, L) = U_4(R, 2L)$, *i.e.* the value of R at which $U_4(R, L)$ and $U_4(R, 2L)$ cross and $U_4^c(L)$ the value of U_4 at the crossing. Similarly $R = R_{c,\xi}(L)$ is the crossing point of $\xi(R, L)/L$, *i.e.* $\xi(R, L)/L = \xi(R, 2L)/2L$ and $\xi^c(L)/L$ the value of $\xi(L)/L$ at the crossing. According to the renormalization group, for large L , $R_{c,U}(L)$ and $R_{c,\xi}(L)$ should converge to the same value R^c which is the critical value of R . Finite size scaling implies

$$R_{c,U}(L) \rightarrow R^c + a_U L^{-1/\nu-\omega}; \quad R_{c,\xi}(L) \rightarrow R^c + a_\xi L^{-1/\nu-\omega} \quad (4)$$

where ν is the correlation length exponent and ω the exponent of the first non leading correction to scaling.

Similarly $U_4^c(L) \rightarrow U_4^c + b_U L^{-\omega}$; $\xi^c(L)/L \rightarrow \xi^c/L + b_\xi L^{-\omega}$. U_4^c , ξ^c/L and the exponents ν and ω are universal quantities.

We will show now the existence of discontinuities of the ground state magnetization as a function of the ratio R . These discontinuities will affect the determination of the crossing points, mentioned above. We illustrate these discontinuities in the case of $d = 0.07$. Large discontinuities

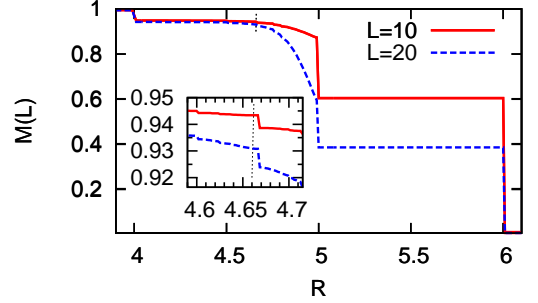


FIG. 1. (Color online.) Magnetization vs. R for the 3D DAFF at $T = 0$ with dilution $d = 0.07$. The inset contains an expansion of the neighbourhood of the critical point.

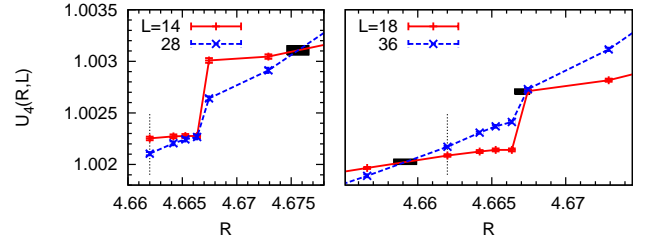


FIG. 2. (Color online.) Crossing of U_4 versus R for the 3D DAFF at $T = 0$ with $d = 0.07$ for $L - 2L = 14 - 28$ and $18 - 36$. The vertical dashed line corresponds to the critical $R^c \simeq 4.662$.

of the magnetization were already observed in the first simulations of the DAFF [13]. They also occur in the 3D RFIM when the probability distribution of the random field is bimodal [3]. In both cases, the position of these discontinuities is independent of the system size L as illustrated below, *i.e.* they don't behave as in eq.(4). They occur when the ratio $R = H_0/J$ goes through a rational number. Because of the dilution, there are spin clusters weakly connected to the rest of the lattice. By changing the value of R it becomes energetically favourable to flip these clusters of spins. This is an artefact of zero temperature. Figure 1 shows the average magnetization as a function of R , for $L = 10$ and $L = 20$. We observe several such discontinuities at values of R which are size independent. The inset of the Figure show the magnetization close to the critical value $R^c \simeq 4.662$ (this value will be determined below). Note that it is very close to a large jump occurring at $R = 14/3 \simeq 4.6666$. This jump corresponds to a change of ground state by flipping clusters of five spins, four spins + and one spin -, $\Delta M = 6$ with a breaking of 14 bonds. The jump of the magnetization will also affect other quantities, in particular $U_4(R, L)$.

In Figure 2, we show the crossings of $U_4(R, L)$ versus R for two pairs of sizes $L - 2L$. In each case we observe again a jump of $U_4(R, L)$ for $R = 14/3$. Since this value is very close to the critical value for R , it will affect the measurements. In particular there can be more than one crossings of $U_4(R, L)$ and $U_4(R, 2L)$. In Figs. 4-5, we show both crossings.

In order to get rid of those spurious singularities a gaussian random component of small amplitude dh_i was added to the external field H_0 [13], *i.e.*

$$H_i = H_0(-1)^{i_x+i_y+i_z} + dh_i, \quad dh_i = wh_i.$$

h_i are independent gaussian random variables of mean zero and variance one and w is the strength of this additional quenched disorder. In both cases of the RFIM with bimodal field distribution and the DAFF the size independent spurious singularities disappear with the addition of dh_i . We will now argue on renormalization group arguments, that in the case of the DAFF, this additional disorder may change the universality class. First consider the Ising antiferromagnet in a field without any dilution or disorder. The Landau-Ginsburg-Wilson Hamiltonian is

$$\begin{aligned} \mathcal{H} = & -J \sum_{\langle xy \rangle} \phi(\vec{x})\phi(\vec{y}) \\ & -H_0 \sum_{\vec{x}} (-1)^{i_x+i_y+i_z} \phi(\vec{x}) - g \sum_{\vec{x}} \phi(\vec{x})^4. \end{aligned} \quad (5)$$

We separate even and odd sites by defining $\psi_{\pm}(\vec{x}) = \phi(\vec{x})(1 \pm (-1)^{i_x+i_y+i_z})/2$. In terms of the new variables $\sum_{\vec{x}} (-1)^{i_x+i_y+i_z} \phi(\vec{x}) = \sum_{\vec{x}} (\psi_+(\vec{x}) - \psi_-(\vec{x}))$ and

$$\begin{aligned} \mathcal{H} = & -J \sum_{\langle xy \rangle} (\psi_+(\vec{x})\psi_-(\vec{y}) + \psi_-(\vec{x})\psi_+(\vec{y})) \\ & -H_0 \sum_{\vec{x}} (\psi_+(\vec{x}) - \psi_-(\vec{x})) \\ & -g(\psi_+^4(x) + \psi_-^4(x) + 2(\psi_+^2(x)\psi_-^2(x))). \end{aligned} \quad (6)$$

This Hamiltonian has the symmetry $\psi_+(\vec{x}) \rightarrow -\psi_-(\vec{x})$ and $\psi_-(\vec{x}) \rightarrow -\psi_+(\vec{x})$, *i.e.* $\phi(\vec{x}) \rightarrow -\phi(\vec{x})$. At the phase transition this symmetry is broken with the appearance of a spontaneous magnetization, while the field $\psi_+(\vec{x}) - \psi_-(\vec{x})$ is non critical and decouples. In other words the antiferromagnet in a constant field in a cubic lattice belongs to the universality class of the ferromagnetic Ising model. By adding a quenched random component to H_0 we change universality class to the one of the RFIM. This is true in the absence of any dilution. We have verified numerically that this is true.

In this paper we consider both cases of $w = 0.1H_0$ and $w = 0.0$. We found that both models are in the same universality class as the RFIM.

We first present our results when a small random field is added to H_0 . We studied the case of $d = 0.07$,

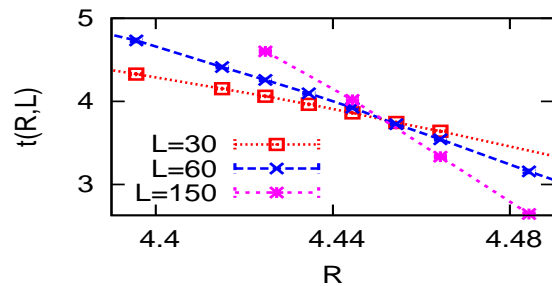


FIG. 3. (Color online.) $t(R, L)$ vs. R for the DAFF with dilution $d = 0.07$ and $T = 0$ in a noisy external field.

$H_0 = 1.0$ and $w = 0.1$. For every sample we compute the ground state magnetization m for different values of the ratio R . We compute the magnetic cumulant U_4 defined above and in order to take into account the constrain $1 \leq U_4(R, L) \leq 3$ we change variables $x(R, L) = (3 - U_4(R, L))/2$, $0 \leq x(R, L) \leq 1$ and $\tanh(t(R, L)) = x(R, L)$. In Figure 3 we show $t(R, L)$ as a function of R and $L \geq 30$. We find that the data are compatible with the finite size scaling hypothesis $t(R, L) = F((R - R^c)L^{1/\nu})$, without needing subdominant corrections in L . We fit the data with the ansatz

$$\begin{aligned} t(R, L) = & F((R - R^c)L^{1/\nu}) = t_0 + t_1(R - R^c)L^{1/\nu} \\ & + t_2(R - R^c)^2L^{2/\nu} + t_3(R - R^c)^3L^{3/\nu}, \end{aligned}$$

valid for $R \simeq R^c$. We found $R^c = 4.4516(50)$, $\nu = 1.43(14)$, $U_4 = 1.0021(9)$ in excellent agreement with Fytas and Martin-Mayor [5] who found for the RFIM $U_4 = 1.0011(18)$ and $\nu = 1.38(13)$. We conclude that our data are compatible with the statement that the DAFF with $H_i = H_0 + dh_i$ is in the same universality class with the RFIM, *i.e.* the addition of dilution does not change the universality class in this case.

Next we present our results when $dh_i = 0$, *i.e.* constant external field with no addition of a random component. For different sizes L and different values of R we compute the following dimensionless ratios $X(R, L)$. $X(R, L)$ is $U_4(R, L)$ or $\xi(R, L)/L$. These are the same quantities considered in [5] and it will allow a direct comparison of our results with those of the RFIM. In order to determine the critical value of R^c , we compute the crossing value $R_X(L)$ of R for which $X(2L) = X(L) = X_c(L)$ and the value $X_c(L)$ at the crossing as explained above. Renormalization group predicts that $\lim_{L \rightarrow \infty} X_c(L)$ is universal.

The results of the crossing for increasing linear sizes L are shown in Figure 4 for the values of dilution, $d = 0.07$ and 0.37 . The lines are linear extrapolations between crossings. We observe two crossing points for some values of L , resulting in the doubling of some sections of the lines in the graph. This is due to the discontinuities of the magnetization discussed above. In both cases, the convergence is very fast. The doubling generates a

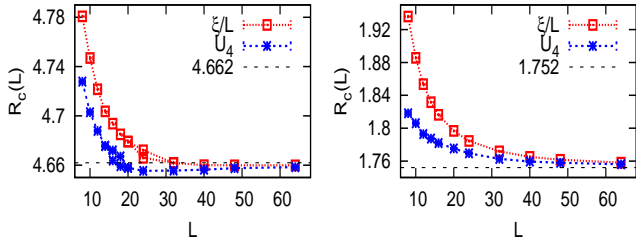


FIG. 4. (Color online.) $R_c(L)$ as a function of L for the correlation length ξ/L and U_4 . The left part corresponds to the dilution $d = 0.07$ and the right part to $d = 0.37$.

small uncertainty in the extrapolation to $L \rightarrow \infty$ which is taken into account in the error bars. We see that $R_{U_4} - R_{\xi/L}$ converges to zero very fast with L . Non leading corrections to the large volume limit are negligible and we can easily extrapolate to $L \rightarrow \infty$. We find $R^c = 4.662(1)$ for $d = 0.07$ and $R^c = 1.752(2)$ for $d = 0.37$ and $R^c = 4.8875(10)$ for $d = 0.05$ (not shown here).

Figure 5 shows the values of U_4 and ξ/L at the crossings for increasing sizes L . We observe that each of these quantities converges nicely toward their asymptotic limit. These limits are compatible to be dilution independent. We determined the asymptotic values $U_4 = 1.0020(5)$ and $\xi/L = 8.5(5)$. The convergence is slower for the dilution probability $d = 0.37$. The existence of multiple crossing points is again visible in the plots but affects very little the asymptotic values, which are fully compatible with those of the 3d RFIM [5] and this for all the three dilution considered. The values for the RFIM are shown in the figures as dashed lines. The middle one corresponds to the value determined in [5] and the two other ones show the upper and lower error bars.

Perturbative renormalization group correctly describes universality classes. The agreement is very good for U_4 and ξ/L .

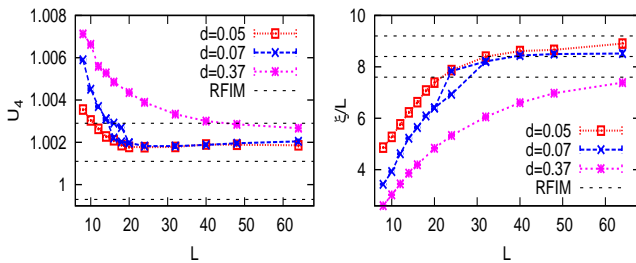


FIG. 5. (Color online.) Crossing of U_4 (left part) and of ξ/L (right part) for the AF 3D IM with dilution $d = 0.05, 0.07, 0.37$ and $T = 0$.

These results make us confident that the DAFF belongs to the same universality class with the RFIM. We assume that this is the case and that the magnetic susceptibility exponent γ and ν take their RFIM values

[5, 21] $\gamma/\nu = 1.48$ and $1/\nu = 0.7$. As in [21], we have applied small additional translation invariant magnetic fields δh_k , $k = 1, 2, \dots$ and change the ferromagnetic coupling to $j_c - dj$. dm_k is the variation of the ground state magnetization m_k due to δh_k and dj . We have computed the probability distribution $P(dm, dj, \delta h, L)$ of dm_k for different values of $dj, \delta h$ and L . In Fig 6

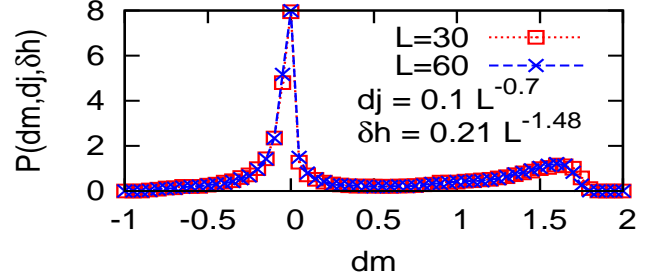


FIG. 6. (Color online.) $P(dm, dj, \delta h)$ vs. dm for $L = 30$ and 60 for $p = 0.07$ and $w = 0.1$.

we show $P(dm, dj, \delta h, L)$ where we simultaneously scale $dj = 0.1L^{-0.7}$ and $\delta h = 0.21L^{-1.48}$. We observe that this probability distribution indicates a strong violation of self averaging and obeys a perfect finite size scaling. This is exactly what happens in the case of the RFIM [21] and with the same values of the critical exponents. It is consistent with the hypothesis that the exponents γ and ν take the same values as in the RFIM, confirming again universality.

In this paper we study the critical behaviour of the diluted antiferromagnet in a field in three dimensions. Our results are fully compatible with the prediction of the perturbative renormalization group (PRG) that it belongs to the same universality class with the random field Ising model. The PRG prediction is for small dilution. It is quite remarkable that a dilution as small as $d = 0.05$ changes the critical values so much, in agreement with PRG. We remind that for the 3D Ising ferromagnet [22] $U_4 = 1.60361(1)$ and $\nu = 0.63002(10)$. We found that universal quantities do not depend on d up to the largest value of d we studied, $d = 0.37$.

There are two very important points we still do not understand : i) Why the perturbative renormalization group predicts correctly universality classes, a highly non trivial prediction, while it fails so much in the prediction of critical exponents (no dimensional reduction). ii) Why numerical simulations do not agree with the experimental results [16–18]. Is this due to the difficulty to equilibrate experimental samples ?

Further studies are required to elucidate these two points.

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